NRMolCol: Inelastic Scattering Data for (exo)Planetary Atmospheres

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The study of molecular scattering is an essential step for understanding a large number of phenomena, from the dynamics and evolution of planetary and exoplanetary atmospheres, the population evolution in plasmas, to the understanding of spectral broadening observed during retrievals [1]. The importance of this field is evident from the vast number of computational methodologies developed over the years (from full quantum methodologies, to quasi classical trajectories, passing by semiclassical approaches) [2]. and the existence of well-recognised databases in the community (KIDA, BaseCol, etc) [3].

This contribution will present the progress made in the improvement of the semiclassical approach (full quantum vibrations, classic rotation and translation) introduced by Billing [4], extending the range of applications of the code (introduction of different functionalities that allows the treatment of rotational-dependent cross sections, etc...), and improving the code performances (different parallelisations schemes, GPU porting...).

Our code is tested against full quantum simulations, using CS+He as a test case [5]. CS has been observed in a variety of objects such as carbon-rich stars, star forming regions, dense interstellar clouds, and recently proposed as sulphour bearing species in WASP-39b [6]. We found that the difference in rates between the two models is within the accuracy of the two approaches. We explored the convergences of our results when changing the number of vibrational states and the number of classic trajectories. We will extend the range of available data to cover the vibrational ladder up to dissociation.

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